

Effective field theory for the $\text{SO}(n)$ bilinear-biquadratic spin chain

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We present a low-energy effective field theory to describe the $\text{SO}(n)$ bilinear-biquadratic spin chain. We start with $n = 6$ and construct the effective theory by using six Majorana fermions. After determining various correlation functions we characterize the phases and establish the relation between the effective theories for $\text{SO}(6)$ and $\text{SO}(5)$. Together with the known results for $n = 3$ and 4, a reduction mechanism is proposed to understand the ground state for arbitrary $\text{SO}(n)$. Also, we provide a generalization of the Lieb-Schultz-Mattis theorem for $\text{SO}(n)$. The implications of our results for entanglement and correlation functions are discussed.

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Introduction.— The study of quantum spin chains dates back to the early days of quantum mechanics [1]. With seemingly simple Hamiltonians, quantum spin chains contain very rich physics and thus attract a considerable interest. A prominent example is the bilinear-biquadratic spin chain with $\text{SO}(n)$ symmetry,

$$H = \cos \theta \sum_j \sum_{a < b} L_j^{ab} L_{j+1}^{ab} + \sin \theta \sum_j \left(\sum_{a < b} L_j^{ab} L_{j+1}^{ab} \right)^2. \quad (1)$$

In the above expression L^{ab} ($1 \leq a < b \leq n$) are the generators of $\text{SO}(n)$ in the n -dimensional vector representation, with the Casimir operator normalized at every site as $\sum_{a < b} (L_j^{ab})^2 = n - 1$. Thus, Eq. (1) represents a family of Hamiltonians parametrized by $\theta \in [-\pi, \pi]$ and n . As an example, the case of $n = 3$ corresponds to the well-known spin-1 bilinear-biquadratic model, of great relevance in the context of Haldane's conjecture [2]. Also, for $n = 4$ the model is equivalent to a symmetrically coupled spin-orbital chain. Such spin-orbital models describe a family of transition metal oxide compounds, where orbital degeneracy plays an important role in the magnetic properties of the material [3]. Quite remarkably, the phase diagram of the model in Eq. (1) for these two cases has been established, and exhibits a rich variety of phases [4–6]. However, the properties for $n \geq 5$ remain mostly unclear yet. For instance, it is unknown whether the behavior in the large- n limit is somehow similar to that of the models with smaller n or not.

In this context, the main contributions of this Letter are (i) to provide a generalization of the Lieb-Schultz-Mattis theorem for $\text{SO}(n)$ and (ii) to present an effective field theory describing the low-energy physics of the model in Eq. (1) for arbitrary n and $\theta \in [0, \theta_{\text{MPS}}]$, with θ_{MPS} a special point to be discussed later. This is relevant since it allows us to understand the low-energy physics of the system in the considered parameter regime *in an exact way*. To achieve this goal, we start with $n = 6$ and show that at a given phase transition point θ_{R} the system is critical and is described by the $\text{SO}(6)_1$ Wess-Zumino-Novikov-Witten model with central charge $c = 3$. This, in turn, allows us to determine various correlation functions characterizing the phases. Then, after

establishing a relationship between the effective theories for $\text{SO}(6)$ and for $\text{SO}(5)$ [7] and gathering some known results for $n = 3$ and 4, we propose a reduction mechanism to understand the ground state of the $\text{SO}(n)$ Heisenberg chain and suggest an effective field theory for Eq. (1) in the considered parameter regime.

Known results for the general $\text{SO}(n)$ case.— Let us now comment briefly on what is known about the model in Eq. (1) for arbitrary n . In Ref. [8] a phase diagram was conjectured based on the existence of some exactly solvable points. For $n \geq 5$, this phase diagram exhibits two remarkable features between the $\text{SO}(n)$ Heisenberg model $\theta_{\text{H}} = 0$ and the integrable $\text{SU}(n)$ Uimin-Lai-Sutherland model $\theta_{\text{ULS}} = \tan^{-1} \frac{1}{n-2}$ [9]. The first one is a parity effect in n ; that is, the physical properties of the system are sharply different if n is even or odd. This is best seen at the special point $\theta_{\text{MPS}} = \tan^{-1} \frac{1}{n}$, where the ground state of the model is exactly described by a matrix product state (MPS) [8, 10, 11]. This MPS is unique and translationally invariant for odd n , whereas it is twofold degenerate and breaks translational symmetry for even n . The second feature is the location of an integrable model at $\theta_{\text{R}} = \tan^{-1} \frac{n-4}{(n-2)^2}$ [12], which sits between θ_{H} and θ_{MPS} for $n \geq 5$. This point turns out also to be critical for all n , which has important implications. For instance, the existence of this point implies that for $n \geq 5$ the MPS point θ_{MPS} no longer captures the physics of the $\text{SO}(n)$ Heisenberg chain. For $n = 5$ this feature is supported by an interesting recent work [7]. Thus, the model in Eq. (1) for $n \geq 5$ has a quite different phase diagram from the $n = 3$ case, where the Affleck-Kennedy-Lieb-Tasaki model at θ_{MPS} qualitatively describes the properties of the spin-1 Heisenberg chain [10].

Generalized Lieb-Schultz-Mattis theorem.— From a general perspective, the parity effect has its roots in the difference of the $\text{SO}(n)$ vector representation for odd and even n . More precisely, for *even* n , there exists an element $g \in \text{SO}(n)$ such that $\exp(i\pi g) = -I_{n \times n}$. The presence of this element enables a generalization of the Lieb-Schultz-Mattis theorem [13]: Assuming that $|\Psi\rangle$ is the unique ground state of the model in Eq. (1), the

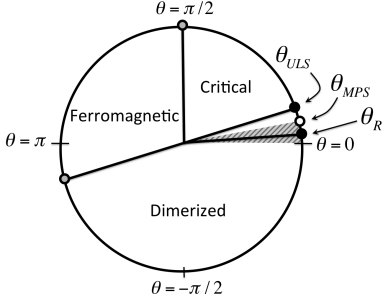


FIG. 1: Predicted phase diagram of the SO(6) bilinear-biquadratic spin chain in Ref. [8]. The shaded area is the region considered in this Letter.

“twisted” state $|\Psi_e\rangle = \exp(i\frac{\pi}{N}\sum_{j=1}^N jg_j)|\Psi\rangle$ is not only orthogonal to $|\Psi\rangle$ but also has a vanishing excitation energy in the thermodynamic limit $N \rightarrow \infty$. This implies that the model with *even* n has either gapless excitations or degenerate gapped ground states with broken translational symmetry. On the contrary, the model with *odd* n can have a unique gapped ground state.

Effective theory for $n = 6$.— Let us consider now the model in Eq. (1) for $n = 6$, whose phase diagram is represented in Fig. 1. Since $\text{SO}(6) \simeq \text{SU}(4)$, this model is equivalent to the SU(4) spin chain with self-conjugate representation **6** in Ref. [14]. For $\theta \in [0, \theta_{\text{MPS}}]$, the conjectured phase diagram in Ref. [14] is in agreement with Ref. [8] and the ground state at θ_{MPS} is identified as an extended valence-bond solid state with broken charge-conjugation symmetry. Moreover, an effective theory was derived in Ref. [14] by using non-Abelian bosonization techniques. Here, though, we use a different approach to obtain an effective theory, which makes a clear connection with the SO(5) effective theory in Ref. [7] and enables a possible extension to general n . As expected, this effective theory recovers the results from Ref. [14].

Following Ref. [15], we derive the field theory for the SO(6) Heisenberg chain by considering the SU(4) Hubbard model in the strong coupling limit. Let us briefly review this approach to make the subsequent discussions self-contained and to introduce some necessary notations. The SU(4) Hubbard model is written as

$$H_{\text{SU}(4)} = -t \sum_{j,\alpha} (c_{j\alpha}^\dagger c_{j+1,\alpha} + \text{H.c.}) + U \sum_j (n_j - 2)^2, \quad (2)$$

where $c_{j\alpha}^\dagger$ is the fermion creation operator at site j with color index $\alpha = 1, \dots, 4$ and $n_j = \sum_\alpha c_{j\alpha}^\dagger c_{j\alpha}$ is the fermion number operator. Here we consider $U > 0$ and the case of a half-filled fermion energy band (two fermions per site). For $U \gg t$, charge excitation is strongly suppressed due to a Mott gap $\Delta_c \sim U$. Thus, two fermions frozen at each site constitute six states $c_\alpha^\dagger c_\beta^\dagger |0\rangle$, which belong to the vector representation of SO(6). In this limit, standard perturbation theory in t/U yields

an SO(6) Heisenberg model [16]. With this correspondence in hand, the SO(6) generators L^{ab} are written as $L^{ab} = \frac{1}{2} \sum_{\alpha\beta} c_\alpha^\dagger T_{\alpha\beta}^{ab} c_\beta$, where the 4×4 SU(4) matrices T^{ab} are normalized as $\text{Tr}(T^{ab} T^{cd}) = 4\delta_{ac}\delta_{bd}$. Since SO(6) is a rank-3 algebra, we choose three diagonal Cartan generators L^{12} , L^{34} , and L^{56} with $T^{12} = \sigma^0 \otimes \sigma^z$, $T^{34} = \sigma^z \otimes \sigma^0$, and $T^{56} = \sigma^z \otimes \sigma^z$, where σ^0 and σ^z are 2×2 identity and Pauli matrices, respectively.

The field theory for the SO(6) Heisenberg chain can be derived by applying Abelian bosonization techniques to the SU(4) Hubbard model (2) [15]. After linearizing the spectra around two Fermi points $k_F = \pm 2\pi/a_0$, the fermion operators are decomposed into left-moving and right-moving components as $c_{j\alpha} \rightarrow \sqrt{a_0}(\psi_{R\alpha} e^{ik_F x} + \psi_{L\alpha} e^{-ik_F x})$, where a_0 is the lattice spacing. These chiral fermions are related to boson fields as $\psi_{R(L),\alpha} = (2\pi a_0)^{-1/2} \zeta_\alpha \exp[\pm i\sqrt{\pi}(\phi_\alpha \mp \Theta_\alpha)]$, where ζ_α are Klein factors. The boson fields for U(1) charge and SO(6) spin channels are just linear combinations of ϕ_α , defined by $\phi_{c,(s_1)} = (\phi_1 \pm \phi_2 + \phi_3 \pm \phi_4)/2$ and $\phi_{s_2,(s_3)} = (\phi_1 \pm \phi_2 - \phi_3 \mp \phi_4)/2$ [6, 17], respectively. Similar equations hold for their dual fields. The bosonized Hamiltonian density $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}$ contains the usual free part $\mathcal{H}_0 = \frac{v_c}{2} [K_c (\partial_x \Theta_c)^2 + \frac{1}{K_c} (\partial_x \phi_c)^2] + \frac{v_s}{2} \sum_{p=1}^3 [K_s (\partial_x \Theta_{s_p})^2 + \frac{1}{K_s} (\partial_x \phi_{s_p})^2]$ with velocities $v_{c,(s)}$ and Luttinger parameters $K_{c,(s)}$. The interaction part is [15] $\mathcal{H}_{\text{int}} = g_s \sum_{p \neq q} \cos \sqrt{4\pi} \phi_{s_p} \cos \sqrt{4\pi} \phi_{s_q} - g_{sc} \cos \sqrt{4\pi} \phi_c \sum_{p=1}^3 \cos \sqrt{4\pi} \phi_{s_p}$, where $g_s, g_{sc} > 0$ and the spin-charge coupling term comes from the $4k_F$ umklapp scattering presence at half filling. Because of the large Mott gap, the charge boson can be safely integrated out. By introducing six Majorana fermions to refermionize the boson fields ϕ_{s_p} , for instance $(\xi^1 + i\xi^2)_{R(L)} \sim \exp[\pm i\sqrt{4\pi} \phi_{s_1,R(L)}]$, the low-energy effective Hamiltonian density describing the SO(6) spin sector reads [15]

$$\mathcal{H}_{\text{eff}} = -\frac{iv_s}{2} \sum_{\nu=1}^6 (\xi_R^\nu \partial_x \xi_L^\nu - \xi_L^\nu \partial_x \xi_R^\nu) - im \sum_{\nu=1}^6 \xi_R^\nu \xi_L^\nu - G_s \sum_{1 \leq \nu < \kappa \leq 6} \xi_R^\nu \xi_L^\nu \xi_R^\kappa \xi_L^\kappa, \quad (3)$$

with $m > 0$ and $G_s > 0$. Equation (3) predicts a gapped ground state with spin-Peierls order for the SO(6) Heisenberg chain [15], which was confirmed numerically [16].

Let us now extend the effective theory in Eq. (3) for the SO(6) Heisenberg chain in order to incorporate a biquadratic interaction. In Eq. (3), the Majorana mass term is relevant and the fermion interaction term is marginally irrelevant for $G_s > 0$. The crucial observation here is that, when the Heisenberg chain is perturbed by the biquadratic interaction, the *only* permitted form of the effective theory is still Eq. (3) but with modified parameters v_s , m , and G_s as functions of θ . The reason for this is that in one spatial dimension only the fermion mass term is relevant and the four-fermion interaction

term is marginal [18]. Other terms are either irrelevant, which play no role in the low-energy limit, or break the $\text{SO}(6)$ symmetry, which is forbidden since the effective theory must preserve the symmetry of the original model.

More evidence for this effective theory comes from the integrable point $\theta_R = \tan^{-1} \frac{1}{8}$ for $n = 6$. The Bethe ansatz solution of this model, as shown by Minahan and Zarembo [19], indicates that there are three branches of gapless excitations above the $\text{SO}(6)$ singlet ground state. In the low-energy limit, these excitations have the same linear dispersion $\varepsilon(p) \simeq v_s p$. This is in full agreement with the effective theory (3) with a vanishing Majorana mass, which becomes the $\text{SO}(6)_1$ Wess-Zumino-Novikov-Witten theory (possibly perturbed by marginally irrelevant terms) with central charge $c = 6 \times \frac{1}{2} = 3$. At this critical point, the “speed of light” v_s in Eq. (3) is given by $v_s = \frac{\pi}{2} \cos \theta_R$, which is determined from the Bethe ansatz solution. For $\theta < \theta_R$, the Majorana mass is expected to be decreasing when θ increases from 0 to θ_R . For $\theta > \theta_R$, it changes sign ($m < 0$) and an energy gap reopens.

Let us now derive the correlation functions. First, we note that the effective theory in Eq. (3) is equivalent to six decoupled Ising models and the Majorana mass is $m \sim (T - T_c)/T_c$ with T_c the Ising critical temperature [20]. For $\theta < \theta_R$, the model in Eq. (1) is in the Ising disordered phase with $\langle \mu_\nu \rangle \neq 0$ ($\nu = 1, 2, \dots, 6$), while for $\theta > \theta_R$ it is in the Ising ordered phase with $\langle \sigma_\nu \rangle \neq 0$ (where μ_ν and σ_ν are the Ising disorder and order operators, respectively). In the continuum limit, the $\text{SO}(6)$ generators are expressed as $L_j^{ab} \simeq J_R^{ab} + J_L^{ab} + (-1)^j n^{ab}$, where the slowly varying $\text{SO}(6)$ Kac-Moody currents $J_{R(L)}^{ab}$ and the staggered components n^{ab} have critical dimensions 1 and $3/4$, respectively. The n^{ab} 's associated with the Cartan generators are $n^{12} \sim \sigma_1 \sigma_2 \mu_3 \mu_4 \mu_5 \mu_6$, $n^{34} \sim \mu_1 \mu_2 \sigma_3 \sigma_4 \mu_5 \mu_6$, and $n^{56} \sim \mu_1 \mu_2 \mu_3 \mu_4 \sigma_5 \sigma_6$. Using all this information, one can see that the two-point correlator $\langle L_j^{ab} L_{j+r}^{ab} \rangle$ decays exponentially in both Ising disordered and ordered phases, while at the critical point θ_R it decays algebraically as

$$\langle L_j^{ab} L_{j+r}^{ab} \rangle \simeq \frac{C_1}{r^2} + (-1)^r \frac{C_2}{r^{3/2}}, \quad (4)$$

where C_1 and C_2 are nonuniversal constants. Furthermore, in Ref. [14], a dimerization operator $\mathcal{D}_j = (-1)^j \sum_{a<b} L_j^{ab} L_{j+1}^{ab}$ and an operator $\mathcal{C}_j = (-1)^j \sum_{a<b} L_j^{ab} L_{j+1}^{ab} L_{j+2}^{ab}$ characterizing the staggered charge-conjugation order were suggested to distinguish between the two phases. Remarkably, in the continuum limit we find that $\mathcal{D} \sim \mu_1 \mu_2 \mu_3 \mu_4 \mu_5 \mu_6$ and $\mathcal{C} \sim \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \sigma_6$, satisfying $\langle \mathcal{D}_i \rangle \neq 0, \langle \mathcal{C}_i \rangle = 0$ for $\theta < \theta_R$ and $\langle \mathcal{D}_i \rangle = 0, \langle \mathcal{C}_i \rangle \neq 0$ for $\theta > \theta_R$, which indeed characterizes the two different phases. At the critical point θ_R these competing orders have the same critical exponents and we have $\langle \mathcal{D}_j \mathcal{D}_{j+r} \rangle \sim 1/r^{3/2}$ and $\langle \mathcal{C}_j \mathcal{C}_{j+r} \rangle \sim 1/r^{3/2}$. Therefore, the critical ground state at θ_R is an algebraic

spin liquid unifying the dimerization order, the staggered charge-conjugation order, and the Néel order.

For the solvable point θ_{MPS} , it was shown in Ref. [8] that the MPS has a hidden antiferromagnetic order quantified by a generalized den Nijs-Rommelse string order parameter (SOP) [21] $\mathcal{O}^{ab} = \lim_{|k-j| \rightarrow \infty} \langle L_j^{ab} \prod_{l=j}^{k-1} \exp(i\pi L_l^{ab}) L_k^{ab} \rangle$. Because of the unbroken $\text{SO}(6)$ symmetry, all these SOPs are equal and it is sufficient to consider the SOPs for the Cartan generators. We find that they are related to the Ising variables as

$$\mathcal{O}^{12} \sim \langle \sigma_1 \rangle \langle \sigma_2 \rangle, \quad \mathcal{O}^{34} \sim \langle \sigma_3 \rangle \langle \sigma_4 \rangle, \quad \mathcal{O}^{56} \sim \langle \sigma_5 \rangle \langle \sigma_6 \rangle \quad (5)$$

These SOPs have nonzero values in the Ising ordered phase for $\theta > \theta_R$ and vanish in the disordered phase for $\theta < \theta_R$. Therefore, they are also proper order parameters for the phase with staggered charge-conjugation order and their utility goes beyond the solvable point θ_{MPS} .

Reduction from $n = 6$ to $n = 5$.— In the following we establish a relationship between the effective field theories for $\text{SO}(6)$ and for $\text{SO}(5)$ [7]. Let us go back to the $\text{SU}(4)$ Hubbard model in Eq. (2) and interpret the fermion color index as spin- $\frac{3}{2}$ quantum numbers ($\alpha = \pm\frac{3}{2}, \pm\frac{1}{2}$). Then, the $\text{SO}(6)$ vector representation at each site unifies the spin-2 quintet states and the spin-0 singlet state formed by two spin- $\frac{3}{2}$ fermions. If an on-site spin-dependent interaction $V \sum_i \mathbf{S}_i^2$ is added to the model (2), then the singlet and quintet sectors pick up different energies and the $\text{SU}(4)$ symmetry of the Hamiltonian is broken down to $\text{SO}(5)$ [22], with an energy difference $\Delta_s \sim V$ between the two sectors. For $V < 0$ the quintet states, forming $\text{SO}(5)$ vector representation, have lower energy and the effective exchange Hamiltonian in the Mott regime is an $\text{SO}(5)$ Heisenberg model [22, 23]. In the field theory treatment [7], the quintet and singlet degrees of freedom are described by Majorana fermions ξ^ν ($\nu = 1 \sim 5$) and ξ^6 , respectively. In Eq. (3), the energy difference Δ_s is formally accounted for by giving ξ^6 a large mass $m_s \gg m_q > 0$, where m_q is the mass of the other five Majorana fermions. In the low-energy limit, integration over ξ^6 yields five massive Majorana fermions with a renormalized mass $m'_q > 0$. Although the five remaining Majorana fermions have a *smaller* mass $m'_q < m_q$, the $\text{SO}(5)$ Heisenberg chain is still in the Ising disordered phase, corresponding to dimerized ground states [7].

Thanks to this mechanism, we can now study the correlation functions of the $\text{SO}(5)$ model. This is accomplished by simply replacing the Ising variables μ_6 and σ_6 in the expressions for $\text{SO}(6)$ by their expectation values $\langle \mu_6 \rangle \neq 0$ and $\langle \sigma_6 \rangle = 0$, respectively. In the $\text{SO}(5)$ Ising ordered phase, unlike the $\text{SO}(6)$ case, translational symmetry is preserved and all two-point correlation functions decay exponentially. For example, it is easy to show that for $\text{SO}(5)$ the operator \mathcal{C} has a vanishing expectation value. However, according to Eq. (5), the nonlocal SOPs

are still nonzero and thus are valid order parameters in this phase.

Reduction and effective theory for arbitrary n .—Motivated by the above discussions, we now propose a reduction mechanism to understand the ground state of the $\text{SO}(n)$ Heisenberg model. As we have seen, the $\text{SO}(n)$ Heisenberg models for $n = 6$ and 5 are both described by n massive Majorana fermions with mass $m > 0$ and marginally irrelevant terms. Formally speaking, one can say that we go from an effective theory for $\text{SO}(n)$ to an effective theory for $\text{SO}(n-1)$ by giving a large mass to the Majorana fermion ξ^n and integrating it out. Because of the marginally irrelevant couplings in the $\text{SO}(n)$ effective theory, the elimination of the large-mass Majorana fermion induces a *negative* contribution to the mass of the $n-1$ remaining Majorana fermions. Usually, the exact values of the parameters in these effective theories are not known. However, the subtlety here is that the $\text{SO}(4)$ Heisenberg chain lies exactly at the critical point θ_R . Since $\text{SO}(4) \simeq \text{SU}(2) \times \text{SU}(2)$, the $\text{SO}(4)$ Heisenberg chain is equivalent to two decoupled spin- $\frac{1}{2}$ Heisenberg chains, whose effective theory contains four *massless* Majorana fermions [24]. Thus, if one wishes to construct this theory from the effective theory for $\text{SO}(5)$, the only possibility to obtain the zero mass of the four Majorana fermions is the miraculous *exact cancellation* of their original mass [in the $\text{SO}(5)$ theory] and the negative contribution that comes from integrating over the large-mass Majorana fermion ξ^5 . We can proceed further from this massless $\text{SO}(4)$ theory on to an $\text{SO}(3)$ theory, where three massive Majoranas with $m < 0$ are obtained and which recovers Tsvetlik's theory for the spin-1 Heisenberg chain [25].

What about the effective field theory for general n ? By combining the results for $n = 3, \dots, 6$ and applying the reduction mechanism in the reverse direction, we can argue that at the integrable point θ_R the $\text{SO}(n)$ spin chain in Eq. (1) is described by an $\text{SO}(n)_1$ Wess-Zumino-Novikov-Witten model with n massless Majorana fermions perturbed by marginally irrelevant terms. This theory has central charge $c = n \times \frac{1}{2}$, and thus the entanglement entropy of a block increases linearly with n for the ground state of the system close to and at θ_R [26]. For $n \geq 5$, the isolated critical point θ_R separates the region $\theta \in [0, \theta_{\text{MPS}}]$ into an Ising disordered phase for $\theta < \theta_R$ and an ordered phase for $\theta > \theta_R$. By using the results in Ref. [27], n zero-energy Majorana modes η^a ($a = 1 \sim n$) localized at the boundary are obtained from the $\text{SO}(n)$ effective theory for $m < 0$ in a semi-infinite chain and form $\text{SO}(n)$ generators $\Gamma^{ab} = i\eta^a \eta^b$ in spinor representation. Note that the $\text{SO}(n)$ spinor is irreducible for odd n but reducible for even n and contains two subspaces. This explains the appearance of $\text{SO}(n)$ spinor edge states at θ_{MPS} and their crucial differences for even and odd n [8]. Another interesting prediction of our theory is the two-point correlator

$\langle L_j^{ab} L_{j+r}^{ab} \rangle$ at the critical point θ_R . In the continuum limit, the $\text{SO}(n)$ generators L^{ab} are a sum of uniform $\text{SO}(n)$ currents with critical dimension 1 and staggered components with critical dimension $n/8$ (n Ising variables). For $3 < n < 7$, the contribution from the staggered components is dominant in the correlator and we have $\langle L_j^{ab} L_{j+r}^{ab} \rangle \sim (-1)^r / r^{n/4}$. However, for $n > 8$, the contribution from uniform $\text{SO}(n)$ currents becomes dominant and in this case $\langle L_j^{ab} L_{j+r}^{ab} \rangle \sim 1/r^2$.

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